Discriminants *à la Sturm* for families of affine sections of positive toric varieties

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I. Introduction

What is a (non-minimal) discriminant?

Informal definition

- A *discriminant* Δ of a parametric family of semialgebraic systems, Σ, is an algebraic object which encodes where in the parameter space Σ does not show generic behaviour.
- Thus Δ can be represented by a semialgebraic set in the parameters.
- The *discriminant variety*, $\mathbb{V}(\Delta)$, of Σ is the zero locus of Δ.
- When $\mathbb{V}(\Delta)$ is a hypersurface, we can take its Zariski closure, and define thus an algebraic discriminant $\tilde{\Delta} = \mathbb{I}(\mathbb{V}(\Delta))$.
- We can also define non-minimal (often, simpler) discriminants by considering any hypersurface containing $\mathbb{V}(\Delta)$.
- Examples of (non-minimal) discriminants are obtained from CADs.

Mathematical motivation

Consider a parametric family of polynomial ODE systems:

$$\begin{aligned}\dot{x}_1 &= P_1(k_1, \ldots, k_r; x_1, \ldots, x_n),\\ &\vdots\\ \dot{x}_n &= P_n(k_1, \ldots, k_r; x_1, \ldots, x_n),\end{aligned}$$

where $k_1, \ldots, k_r \in \mathbb{R}_{>0}$ are parameters, $x_1 > 0$, …, $x_n > 0$, and

$$P_i \in \mathbb{R}(k_1, \ldots, k_r)[x_1, \ldots, x_n] \text{ or } P_i \in \mathbb{R}[k_1, \ldots, k_r][x_1, \ldots, x_n]$$

are polynomials in $x_1, \ldots, x_n$ and rational/polynomials in $k_1, \ldots, k_r$.

Problem 0

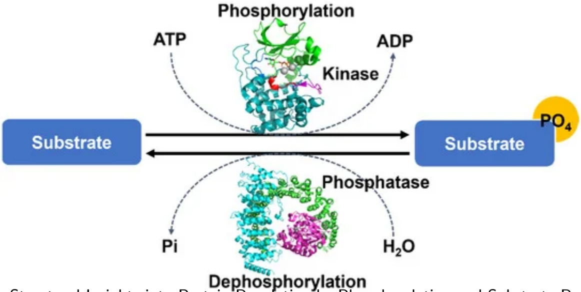
Study the steady states of the previous ODE system, that is, solve the semialgebraic system $\dot{x}_i = 0$, $x_i > 0$, $i = 1, \ldots n$.

Biological motivation

The following network is the sequential distributive 2-site phosphorylation:

$$S+K \underset{k_2}{\overset{k_1}{\rightleftarrows}} SK \xrightarrow{k_3} S_p+K \underset{k_5}{\overset{k_4}{\rightleftarrows}} S_pK \xrightarrow{k_6} S_{pp}+K$$

$$S_{pp}+P \underset{k_8}{\overset{k_7}{\rightleftarrows}} S_{pp}P \xrightarrow{k_9} S_p+P \underset{k_{11}}{\overset{k_{10}}{\rightleftarrows}} S_pP \xrightarrow{k_{12}} S+P$$



[Source: Seok, S.-H. Structural Insights into Protein Regulation by Phosphorylation and Substrate Recognition of Protein Kinases/Phosphatases. Life 2021, 11, 957]

Steady states – algebra dictionary

Definition

- Each positive solution: *positive steady state*.
- The set of all solutions (k, x): *positive steady state variety*, V^+.
- The ideal generated by these polynomials: *steady state ideal*.

Definition (2016; Müller, Feliu, Regensburger, Conradi, Shiu, Dickenstein)

V^+ is *positive toric* if $\exists M \in \mathbb{Z}^{n\times d}$ of rank $p < n$ and a rational function

$$\begin{array}{rccc} \gamma: & \mathcal{K}_\gamma^+ & \to & \mathbb{R}^d \\ & k & \mapsto & \gamma(k), \end{array}$$

such that $(k, x) \in V^+ \Leftrightarrow x^M = \gamma(k) \quad \forall (k,x) \in \mathcal{K}_\gamma^+ \times \mathbb{R}^n_{>0}$, where $\mathcal{K}_\gamma^+ = \left\{k \in \mathbb{R}^r_{>0} \mid \gamma_i^+(k)\, \gamma_i^-(k) > 0,\ i \in [d]\right\}$ and $\gamma_i^\pm(k) \in \mathbb{R}[k]$ are such that $\gamma^\pm(k) = \left(\gamma_1^\pm(k), \ldots, \gamma_d^\pm(k)\right)$, where $\gamma_i(k) = \frac{\gamma_i^-(k)}{\gamma_i^+(k)}$ for $i \in [d]$.

Informally: V^+ is positive toric if $\overline{\mathbb{V}(I_k) \cap \mathbb{R}^n_{>0}}$ is generically nonempty toric.

Problem 1

Find the (real/complex) **steady state variety**, that is, solve the polynomial system $\dot{x}_1 = \ldots = \dot{x}_n = 0$ for complex/real $x_1, \ldots, x_n$.

Problem 1'

Find the largest $\mathcal{K}_\gamma^+ \subset \mathbb{R}_{>0}^r$ such that, whenever $(k_1, \ldots, k_r) \in \mathcal{K}_\gamma^+$, the polynomial system $\dot{x}_1 = \ldots = \dot{x}_n = 0$ has positive solutions $x_1, \ldots, x_n$.

Problem 1''

Add to Problem 1/1' restrictions derived from conservation laws.

Problem 2

Classify all (or some) of the parameters $k_1, \ldots, k_r$ and the conserved quantities $c_1, \ldots, c_s$ with respect to the **existence** of multiple steady states.

Problem 2' (The Discriminant – This Talk)

Classify all parameters $k_1, \ldots, k_r$ and the linear conserved quantities $c_1, \ldots, c_s$ with respect to the **number** multiple steady states.

One possible solution to Problem 1'

Quantifier elimination (¿via CADs?) for

$\exists x_1, \dots x_n \in \mathbb{R}$ such that

$P_1 = 0, \dots, P_n = 0,\ k_1 > 0, \dots, k_r > 0,\ x_1 > 0, \dots, x_n > 0.$

Example of Problem 1'

$$\begin{cases} \dot{x} &= ax^2 + bx + c \\ \dot{y} &= -ax^2 - bx - c \end{cases}, x > 0, y > 0, a > 0, b > 0, c > 0.$$

Then, the quantified statement

"$\exists x, y \in \mathbb{R}$ such that :
$ax^2 + bx + c = 0 \wedge -ax^2 - bx - c = 0$
$\wedge a > 0 \wedge b > 0 \wedge c > 0$
$\wedge x > 0 \wedge y > 0$"

is equivalent to quantifier free statement

$$a > 0 \wedge b > 0 \wedge c > 0 \wedge b^2 - 4ac \geq 0 \wedge ac < 0$$

which is equivalent to the easier quantifier free statement

FALSE

A (NAÏVE) solution to Problem 2'

- Let I be the ideal generated by $P_1, \dots, P_n$ and the conservation laws.
- Compute all elimination ideals $I_i := I \cap \mathbb{R}[k_1, \dots, k_r, c_1, \dots, c_s, x_i]$.
- Assume $\mathbb{V}(I)$ is generically zero dimensional and I_i is principal nonzero.
- Use Sturm sequences to compute a discriminant for $\mathbb{V}(I_i)$.
- Leave the conference room: computationally intractable (and not new).

Remark (Negative aspects)

- Be careful with the word "generic".
- Elimination ideals are problematic (extra solutions in $\mathbb{C}$ or at ∞). This makes the discriminant non-minimal. Not apropiate in Real Algebra?

Remark (Positive aspects)

- Sturm sequences count the number of roots without multiplicity.
- We only count positive roots: we only need the LC and the CT of the Sturm sequences. (This drops the degree of the discriminant).
- Using monomial parameterizations: reduces the complexity a lot.

II. Parametric families
of affine sections of positive toric varieties

Assume linear conservation laws are $Zx = c$, where c are parameters. This works with any *affine linear sections*. We can also add non-linear restrictions.

Theorem (Conradi, I., Kahle; 2018)

Let V^+ be positive toric with exponent matrix A and let $\psi(k) \star \xi^A$ be its monomial parameterization. Then the following are equivalent:

i. $\exists k \in \mathcal{K}_\gamma^+$ and $a \neq b \in \mathbb{R}^n_{>0}$ such that $(k, a), (k, b) \in V^+$, and $Za = Zb$,

ii. $\exists k \in \mathcal{K}_\gamma^+$, $\xi_1 \neq \xi_2$ and c such that $Z(\psi(k) \star \xi_1^A) = Z(\psi(k) \star \xi_2^A) = c$.

Theorem (Conradi, I., Kahle; 2018)

Let V^+ be positive toric with exponent matrix A, let $g_1, \dots, g_l \in \mathbb{R}[c]$, $\square \in \{>, \geq\}^l$, and $\mathcal{F}(g(c) \square 0)$ be any logical combination of the inequalities $g(c) \square 0$. Then, the following are equivalent:

i. $\exists k \in \mathcal{K}_\gamma^+$ such that there is multistationarity in the region defined by $\mathcal{F}(g(c) \square 0)$,

ii. $\exists a \in \mathbb{R}^n_{>0}$, $\xi \neq \mathbf{1}$ such that $Z(a \star \xi^A - a) = 0$ and $\mathcal{F}(g(Za) \square 0)$.

Sturm Discriminants: The univariate case

Let $R = \mathbb{R}[k_1, \dots, k_r]$ and $\mathbb{K} = \mathbb{R}(k_1, \dots, k_r)$. If $p \in R[x]$ is any univariate polynomial, then the *Sturm sequence* $s(p)$ of p is the sequence of signed remainders of p and p', i.e.

$$s(p) = (s_0(p), \dots, s_r(p)) \in (\mathbb{K}[x])^{r+1},$$

where $s_0(p) = p$, $s_1(p) = p'$, $s_i = -\mathrm{Rem}(s_{i-2}(p), s_{i-1}(p))$ for $2 \leq i \leq r$, and r is such that $s_r(p) \neq 0$ and $\mathrm{Rem}\,(s_{r-1}(p), s_r(p)) = 0$.

Definition

The *Sturm discriminant* $\Delta_S(p)$ of $p \in R[x]$ is the polynomial obtained by multiplying the numerators and denominators of the leading coefficients and nonzero constant terms of elements of $s(p)$. Connected components of $\mathbb{R}^m \setminus \mathbb{V}(\Delta_S(p))$ are called cells of the discriminant.

Remark

There might be values of the parameters k for which the specialization of $s(p)$ is not well defined. However, a specialization of the Sturm sequence is always well defined for values of the parameters lying in $\mathbb{R}^m \setminus \mathbb{V}((\Delta_S(p)))$.

Theorem

If $p(0) \neq 0$ and a and b are contained in a common cell of $\mathbb{V}(\Delta_S(p))$, then p_a and p_b have the same number of distinct positive roots.

Definition

A degree d polynomial $p \in R[x]$ is *Sturm generic* if its Sturm sequence has $d + 1$ elements and, for $i \in \{0, \ldots, d\}$, $s_i(p)$ has $d - i + 1$ terms.

Lemma

Sturm generic polynomials exist in any degree.

Proposition

If the coefficients of p are all nonzero and algebraically independent, then p is a Sturm generic polynomial.

Sturm Discriminants: Zero dimensional ideals

Let Σ be a parametric family of multivariate zero dimensional systems of equations and let $I \subseteq R[x_1, \ldots, x_n]$ denote the corresponding ideal. Suppose that I is such that, for all $i \in [n]$, the elimination ideal $I_i = I \cap R[x_i]$ is principal and nonzero). Let $p_i \in R[x_i]$ denote the generator of I_i.

Definition

The *Sturm discriminant* of I is $\Delta_S(I) = (\prod_{i=1}^m \Delta_S(p_i))_{\text{red}}$ and the *Sturm discriminant variety* of I is $\mathbb{V}(\Delta_S(I))$. Connected components of $\mathbb{R}^m \setminus \mathbb{V}(\Delta_S(I))$ are called *cells* of the discriminant.

Theorem

If, for all $i \in [n]$, $p_i(0) \neq 0$ and a and b are contained in a common cell of $\mathbb{V}(\Delta_S(I))$, then the sets $\mathbb{V}(I_a) \cap \mathbb{R}^m_{>0}$ and $\mathbb{V}(I_b) \cap \mathbb{R}^m_{>0}$ have the same number of points.

Proof: The generic case follows from the univariate case. In general, one should be careful with the Extension Theorem, for we work over $\mathbb{R}$. But, since the variety of a projection contains the projection of a variety, at worst, the Sturm discriminant might contain unnecesary extra factors.

III. Implementations and computations

Macaulay2

sturmdiscriminants / **SturmDiscriminants.m2**

```
-- -*- coding: utf-8 -*-
newPackage(
    "SturmDiscriminants",
    Version => "0.1",
    Date => "October 2018",
    Authors => {{
          Name => "Alexandru Iosif",
          Email => "alexandru.iosif@ovgu.de",
          HomePage => "https://alexandru-iosif.github.io"}},
        Headline => "Computation of Sturm Discriminants",
    AuxiliaryFiles => false,
        PackageImports => {"Elimination"},
    DebuggingMode => false
)

export {
     -- 'Official' functions
     "SturmDiscriminant",
     "SturmSequence"
```

Maple

maplesturmdiscriminants / **SturmDiscriminants.mpl**

```
#####
with(PolynomialIdeals):
with(Groebner):
with(Student[MultivariateCalculus]):
with(Student[LinearAlgebra]):
with(combinat):

#####
SturmDiscriminants := module()
description "Sturm Discriminants";
#Author: Alexandru Iosif
option package;


#####
export SturmSequence, SturmDiscriminant, MonomialExponent, areAlgebraicallyIndependent, GenericPolynomial;

```

Example: the 2-site phosphorylation

Dynamics:

$$
\begin{aligned}
[\dot{S}] &= -k_1[S][K] + k_2[SK] + k_{12}[S_pP] \\
[\dot{K}] &= -k_1[S][K] + (k_2 + k_3)[SK] - k_4[K][S_p] + (k_5 + k_6)[S_pK] \\
[\dot{SK}] &= k_1[S][K] - (k_2 + k_3)[SK] \\
[\dot{S_p}] &= k_3[SK] - k_4[K][S_p] + k_5[S_pK] + k_9[S_{pp}P] - k_{10}[S_p][P] + k_{11}[S_pP] \\
[\dot{S_pK}] &= k_4[K][S_p] - (k_5 + k_6)[S_pK] \\
[\dot{S_{pp}}] &= k_6[S_pK] - k_7[S_{pp}][P] + k_8[S_{pp}P] \\
[\dot{P}] &= -k_7[S_{pp}][P] + (k_8 + k_9)[S_{pp}P] - k_{10}[S_p][P] + (k_{11} + k_{12})[S_pP] \\
[\dot{S_{pp}P}] &= k_7[S_{pp}][P] - (k_8 + k_9)[S_{pp}P] \\
[\dot{S_pP}] &= k_{10}[S_p][P] - (k_{11} + k_{12})[S_pP].
\end{aligned}
$$

Conservation laws:

$$[K]+[SK]+[S_pK]=K_{\mathrm{tot}},$$
$$[S_{pp}P]+[S_pP]+[P]=P_{\mathrm{tot}},$$
$$[S]+[S_p]+[S_{pp}]+[SK]+[S_pK]+[S_{pp}P]+[S_pP]=S_{\mathrm{tot}}.$$

The positive steady state variety V^+ admits a monomial parameterization:

$$[S]=\frac{(k_2+k_3)k_4k_6(k_{11}+k_{12})k_{12}}{k_1k_3(k_5+k_6)k_9k_{10}}\frac{\xi_1^2}{\xi_2\xi_3} \qquad [S_pK]=\frac{k_9}{k_6}\xi_2$$

$$[K]=\frac{(k_5+k_6)k_9k_{10}}{k_4k_6(k_{11}+k_{12})}\frac{\xi_2\xi_3}{\xi_1} \qquad [S_{pp}]=\frac{k_8+k_9}{k_7}\frac{\xi_2}{\xi_3}$$

$$[SK]=\frac{k_{12}}{k_3}\xi_1 \qquad [P]=\xi_3$$

$$[S_p]=\frac{k_{11}+k_{12}}{k_{10}}\frac{\xi_1}{\xi_3} \qquad [S_{pp}P]=\xi_2$$

$$[S_pP]=\xi_1$$

where $\xi_1,\ \xi_2,\ \xi_3\in\mathbb{R}_{>0}$.

A note on the parameters we used

Let us use the following notation:

$$
\begin{aligned}
a_1 &:= k_4 k_6 k_7 k_{10} k_{12}(k_2 + k_3),\\
a_2 &:= k_1 k_4 k_6 k_7 k_{10} k_{12},\\
a_3 &:= k_1 k_3 k_4 k_6 k_7 (k_{11} + k_{12}),\\
a_4 &:= k_1 k_3 k_4 k_6 k_7 k_{10},\\
a_5 &:= k_1 k_3 k_7 k_9 k_{10}(k_5 + k_6),\\
a_6 &:= k_1 k_3 k_4 k_7 k_9 k_{10},\\
a_7 &:= k_1 k_3 k_4 k_6 k_{10}(k_8 + k_9).
\end{aligned}
$$

Note that these new parameters are algebraically independent. They were used in [Millan, Dickenstein, Shiu, Conradi, 2012].

A tiny part of the discriminant (in parameters k!!!)

[illegible]

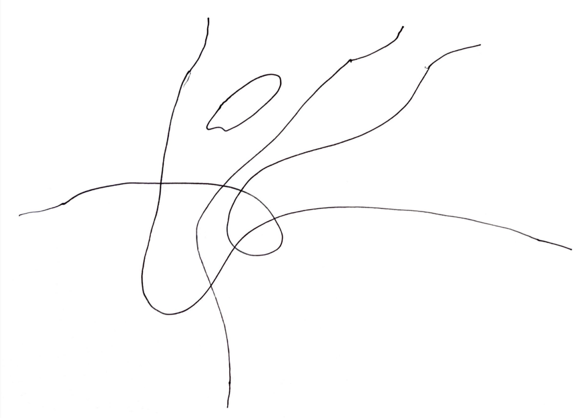
Comments on computations

- M2:
  - elimination step is extremely slow.
  - for free software, maybe try Singular (F4 and F5 algorithms).
- Maple:
  - There is already an implementation based on Lazard and Rouiller. Too demanding and computations do not finish after 6 hours (the output would give more complete information, e.g., cells).
  - In Maple the elimination step is instaneous (due to F4 and F5?).
  - Our algorithm computes a discriminant (Sturm Generic!)
    - huge: 72 factors ($3 \times 6 \times 2 \times 2$.)
    - no information on its cells.
    - nonminimal.
    - positive factors.
- Next steps:
  - Analyze the disciminant and remove positive components.
  - People already computed partial discriminants in this system. Find them.
  - Compute a point in each cell.
  - (Partial) topology of the discriminant? (Zeta functions?)

IV. Divagaciones* poco rigurosas sobre funciones ζ

*Divagación: Dícese de un conjunto de ideas vagas que alguien cree transcribir del Libro.

Consider an algebraic discriminant variety, $\mathbb{V}(\Delta)$, of codimension 1.



How to construct a zeta function for Δ or $\mathbb{V}(\Delta)$ that takes into acount the number of roots, the cells, their topology, etc? **(I do not have an answer)**.

Some zeta functions (possible inspiration places)

$$\zeta(s)=\sum_{n=1}^{\infty}\frac{1}{n^s}=\prod_{p\ \text{prime}}\frac{1}{1-p^{-s}}$$

$$Z(V,s)=\exp\left(\sum_{m=1}^{\infty}\frac{\# V_{\mathbb{F}_{q^m}}}{m}\,(q^{m})\right)$$

$$Z(X\times Y,s)=Z(X,s)*_t Z(Y,s)$$

$$\zeta_\mu(V,t)=\sum_{n\geq 0}\mu\left[\mathrm{Sym}^n(V)\right]t^n\in 1+t\mathbb{R}[[t]]$$

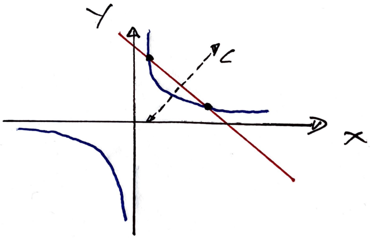
$$Z_{mot}(V,t)=\sum_{n\geq 0}\left[\mathrm{Sym}^n(V)\right]t^n\in 1+K_0\left(\mathrm{Var}/_{\mathbb{R}}\right)[[t]]$$

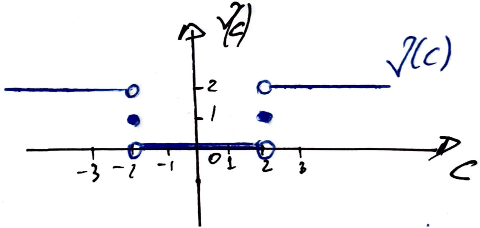
A toy example

Take the following parametric system of equations in $\mathbb{R}[c][x,y]$:

$$V : \begin{cases} xy = 1 \\ x + y = c \end{cases}$$

Its discriminant is $c^2 - 4$, hence V is singular at $c = \pm 2$.
Denote $\nu(c) := \#|V_c|$.





Wide open ideas

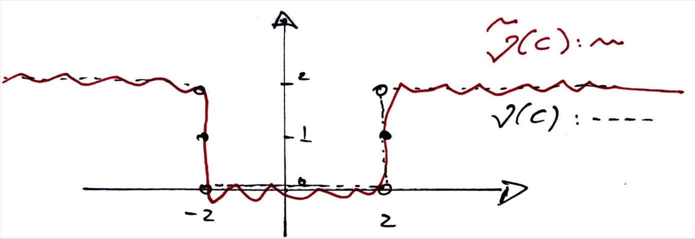
- Since c varies continuously, maybe define a continuous zeta function:

$$\zeta_{\mathrm{CSA}}(V,t) = \int_{-\infty}^{+\infty} f(t,c,\nu(c))\mu(c)dc.$$

- Maybe also define a “continuous” $\tilde{\nu}(c)$ through a Fourier integral:

$$\tilde{\nu}(c) = \int_{-\infty}^{+\infty} \hat{\nu}(k)e^{i2\pi kc}dk.$$

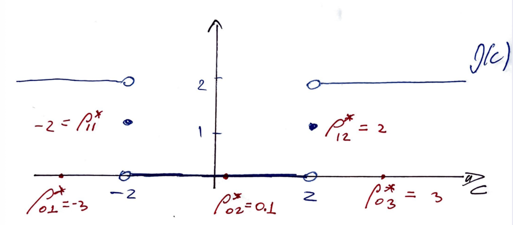
Note that $\tilde{\nu}(c) = \nu(c)$ if $c \in \mathbb{R} \setminus \mathbb{V}(\Delta)$.



Maybe we would like to achieve something like:

$$\zeta_{SA} = \prod_{j=0}^{n}\prod_{i=0}^{\sigma_j}\left(1-\vec{\rho}_{ji}^{\,*}\,t^{j+1}\right)^{(-1)^j(\nu(\rho_{ji})+1)} \overset{\text{Taylor}}{=\!=} \sum_{n=0}^{\infty}\frac{\zeta_{S.A}^{(n)}(0)}{n!}(t-0)^n.$$

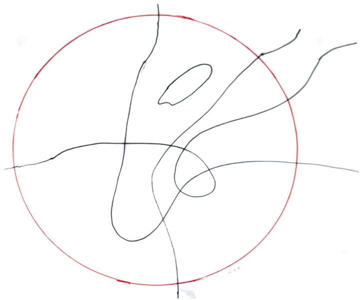
- $\vec{\rho}_{ji}^{\,*}$ is a generic point (avoid cancelations) of ρ_{ji}, the i^{th} cell of codimension j (maybe introduce "ramdomness" in their definition),
- σ_j is the number of codimension j cells,
- In our example:



$$\zeta_{SA} = \frac{(1+3t)^{2+1}(1-0.1t)^{0+1}(1-3t)^{2+1}}{(1+2t^2)^{1+1}(1-2t^2)^{1+1}}. \qquad \text{(Useless?)}$$

Simplicial complexes (towards their zeta functions?)

Take the intersection of $\mathbb{V}(\Delta)$ with a closed ball B of radius "large enough".



$\mathbb{V}(\Delta) \cap B$ is closed and bounded (encodes the shape of the discriminant). Consider all cells ρ_{ji} (any codimension $j \geq 1$), and take a triangulation respecting ρ_{ji}. The triangulation respects the shape of $\mathbb{V}(\Delta) \cap B$.

Let K be a simplicial complex:

- $\mathrm{Ch}_i(K)$ is the $i-$*chain group* of K, that is, $\mathrm{Ch}_i(K)$ is the $\mathbb{R}-$vector space generated by the $i-$dimensional vertices of K,
- $\partial_i : \mathrm{Ch}_i \to \mathrm{Ch}_{i-1}$ and $\delta^i : \mathrm{Ch}^{i-1} \to \mathrm{Ch}^i$: boundary/coboundary maps,
- $L_i = \delta^i \partial_i + \partial_{i+1}\delta^{i+1}$ is the Laplacian map,
- $H_i(K) = \ker\partial_i / \mathrm{im}\partial_{i+1}$ its i^{th} simplicial homology group.

Theorem [Eckmann, 1945 / Duval&Reiner, 2002].

There is an isomorphism of $\mathbb{R}-$vector spaces: $H_i(K) \cong \ker L_i$.

Question

The standard laplacian of the graph (1-skeleton) of K is L_0. The *spectral zeta function* of a graph gives some information about its shape:

$$\zeta_L(t) = \sum_{\lambda \neq 0} \frac{1}{\lambda^t}.$$

What is a version of this zeta function for a simplicial complex?
(Little information in the literature. If you know something, tell me.)

Definition (Ihara zeta function of a graph)

A *prime* $[P]$ in a graph G is an equivalence class of closed paths $e_1 e_2 \ldots e_s$ such that $e_s \neq e_1^{-1}$ and $a_{i+1} \neq a_i^{-1}$ (two walks are equivalent if they are related by a cyclic permutation of vertices). The *Ihara zeta function* of G is

$$\zeta_G(t) = \prod_{[P] \text{ prime}} \frac{1}{1 - t^{|[P]|}}.$$

If we consider weighted lengths $|\cdot|_w$ in G, we can define a weighted version:

$$\zeta_{G,w}(t) = \prod_{[P] \text{ prime}} \frac{1}{1 - t^{|[P]|_w}}.$$

Question

The Ihara zeta function also gives some information about the topology of a graph. How to define it for a simplicial complex (maybe, considering the weights to be the number of roots)? Relation to the spectral zeta function? **(Again, little information in the literature. If you know something...)**

Motivic zeta functions (Comte & Fichou, 2014)

The motivic zeta function for semialgebraic formulas is the most promissing:

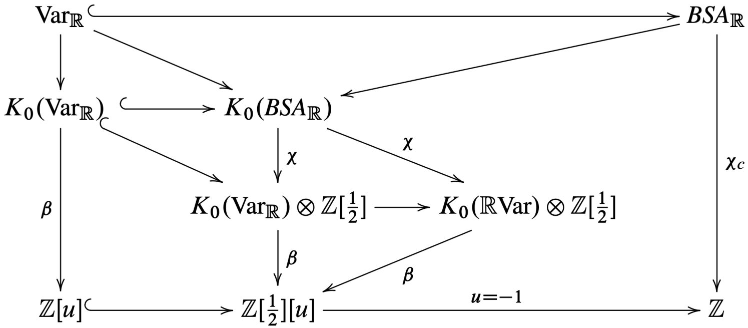


Figure: A commutative diagram. [Source: Comte & Fichou, 2014]

It seems the corresponding motivic zeta function gives a lot a information about the topology of the complementary of a hypersurface, but in a complicated way. **Simplicial complex version (scissor groups for polygons (they have $K_0 = \mathbb{R}$))? Relate to the previous zeta functions?**

Some bibliography

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¡Muchas Gracias!

Vă Mulțumesc!